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Polarizability of a Coulomb-modified potential

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Abstract The dipole polarizability α_d of a Coulomb potential modified by δ/r^2 term has been evaluated in the closure approximation δ is a small positive number In this approximation, $\alpha_d = (2/3) <r^2>/\Delta$ where Δ is the mean excitation energy which is estimated *via* Bethe theory for the stopping cross section for a moving point charge interacting with a bound system. In this approach, only the unperturbed wavefunctions are required to evaluate Δ For this bound system, the values of $<r^2>$ and Δ can be obtained in closed form It is shown that Δ is related to the information-entropy We have found that for the bound system investigated here, α_d increases with δ Behaviour of Δ for small δ is investigated and the correction factors to the hydrogenic problem are found to be in good agreement with the results obtained through a mapping procedure in which the mean excitation energy is taken to be the excitation energy of the first excluded state in the summation over intermediate states in the evaluation of α_d

Keywords Polarizability, mean excitation energy, information entropy

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The electric dipole polarizability α_d is an important property of a bound system. It represents the simplest linear response of the electronic charge cloud of the bound system to an electric field. It is related to the dielectric constant [1]. It is important in the theory of electron or positron scattering from atoms and molecules since the polarization potential behaves as $-\alpha_d/2r^4$ in the asymptotic region [2]. It is also a measure of the Stark shift of energy levels of the bounds system. In optics, it is useful in the analysis of refraction and scattering of light [3].

The evaluation of α_d can be done *via* second-order perturbation theory [4]. It is given by

$$\alpha_d = 2\left| \psi_1^{(1)}, \sum^{N} r_i P_1 (\cos\theta_i) \psi_0 \right|, \tag{1}$$

where ψ_0 is the unperturbed wavefunction and $\psi_1^{(1)}$ is the first-order perturbed wavefunction of the bound system. The summation is over all electrons N of the bound system. Since the

spectrum of hydrogen atom is known exactly, the value of α_d can be computed. Its non-relativistic value is 4.5 a_0^3. However, for a modified Coulomb potential the calculation becomes quite cumbersome. In the present work, we have evaluated α_d for a Coulomb potential $-1/r$ which is modified by an additional term δ/r^2 where δ is a small positive number. In our approach, only the unperturbed wavefunctions are required to evaluate α_d. This approach has been successfully applied to obtain the relativistic correction to α_d of a hydrogenic ion [5].

Eq. (1) can be rewritten by expressing $\psi_1^{(1)}$ over a complete set of unperturbed wavefunctions as

$$\alpha_d = 2 \sum_{n \neq 0} \frac{|\psi_n, \sum^{N} r_i P_1(\cos\theta_i)\psi_0}{E_n - E_0} \tag{2}$$

The summation over n is over all discrete intermediate states and an integration over the continuum. The evaluation of α_d through eq. (2) required a complete knowledge of the full spectrum of the atomic system. A great simplification stems out if we replace the energy denominators by a mean excitation energy Δ. By making use of the completeness relation

$$\sum_{n=0} |\psi_n > < \psi_n| = 1, \tag{3}$$

we get

$$\alpha_d = \frac{1}{\Delta} \left(\psi_0, \sum_{i=1}^{N} r_i^2 P_1^2(\cos\theta_i)\psi_0 \right) - \left(\psi_0, \sum_{i=1}^{N} r_i P_1(\cos\theta_i)\psi_0 \right) \tag{4}$$

We now consider a Coulomb-modified potential

$$V(r) = -\frac{1}{r} + \frac{\delta}{r^2}. \tag{5}$$

The ground-state wavefunction ψ for this bound system has already been obtained [6]. It is given by

$$\psi = \frac{1}{[4\pi\Gamma(2\eta+2)]^{1/2}} \left(\frac{1}{\eta}\right)^{\eta+1} r^{(\eta-\frac{1}{2})} e^{-r/2\eta} \tag{6}$$

where $\eta = \frac{1}{2} + \sqrt{\delta}$.

For the Coulomb-modified potential, eq. (4) can now be written as

$$\alpha_d = \frac{2}{3} \frac{< r^2 >}{\Delta} \tag{7}$$

Using (6), it is trivial to calculate $<r^2>$ which is given by

$$< r^2 > = 2\eta^2(\eta+1)(2\eta+3). \tag{8}$$

Now the main task is to evaluate Δ. It has been shown that [5]

$$2 \ln \Delta = < \ln 4\pi \rho(r) > . \tag{9}$$

Eq. (9) is very important because it determines Δ which is dependent only on the charge density of the electron cloud of the bound system. The average of $\ln 4\pi\rho(r)$ is to be taken over the unperturbed wavefunction. So with this approach, the infinite sum over intermediate states including the integration over the continuum has been replaced by a simple quantity Δ which can be trivially obtained.

It is important to note that eq. (9) can be rewritten as

$$\ln \frac{\Delta^2}{4\pi} = -S, \tag{10}$$

where $S = - < \ln \rho(r) >$ is known as the information entropy [7] for the system with a continuous probability distribution. The use of information entropy is useful in communication networks, analysis of populations and probabilities for many problems. The knowledge of ground state $\rho(r)$ completely determines Δ. This compliments the pivotal role of ground state charge density in the density functional theory [8] which uniquely determines all electronic properties of the system.

Using $\rho(r)$ in eq. (10), we get

$$\Delta = \frac{\exp\left[(\eta - \frac{1}{2})\,\psi(2\eta+2) - (\eta+1)\right]}{\eta^{3/2}\left[\Gamma(2\eta+2)\right]^{1/2}}, \tag{11}$$

where
$$\psi(x) = -C + \sum_{n=0} \left(\frac{1}{n+1} - \frac{1}{x+n} \right) \tag{12}$$

with $C = 0.577215$ is the Euler's constant. Using eqs. (8) and (11) in eq. (7), we finally get

$$\alpha_d = \frac{4}{3}\left[\eta^7\,\Gamma(2\eta+2)\right]^{1/2} (\eta+1)(2\eta+3)\, \exp\left[(\eta+1) - (\eta - \frac{1}{2})\psi(2\eta+2) \right]. \tag{13}$$

It is to be noted that when $\eta = \frac{1}{2}$, our problem reduces to hydrogen atom problem. Eq. (12) yields $\alpha_d = \exp(3/2) = 4.4817\, a_0^3$ which is within half a percent of its exact value $4.5\, a_0^3$. We find that α_d increases with δ due to the presence of the exponential factor. As δ increases, $<r^2>$ increases whereas Δ decreases. This can be easily understood because when δ increases, the bound system becomes loose thereby increasing $<r^2>$ and decreasing the binding energy. Consequently, the energy levels of the system become more compact which results in the decrease of Δ.

It is interesting to evaluate Δ by mapping its value with the hydrogen atom problem. It is knwon that for hydrogen atom, $\Delta = 4/9$ (a.u.) which is the excitation energy of the $3s$ state.

This is the first state which is excluded from the sum over intermediate states. The energy of the E_{1s} state for our present problem is

$$E_{1s} = \frac{-1}{8\left[\frac{1}{2}+\sqrt{\delta}\right]^2}\text{(a.u.)}, \tag{14}$$

whereas $$E_{3s} = \frac{-1}{8\left[\frac{3}{2}+\sqrt{\delta}\right]^2}\text{(a.u.)}. \tag{15}$$

From eqs. (14) and (15), we get

$$\Delta_m = E_{3s} - E_{1s} = \frac{4(1+\sqrt{\delta})}{8\left[3+8\sqrt{\delta}+4\delta\right]^2}\text{(a.u.)}, \tag{16}$$

Δ_m refers to the mapped mean-excitation energy. By using the known properties of $\psi(x)$ and $\Gamma(1+x)$ for $x<1$, we obtain expressions for Δ and Δ_m to order δ,

$$\Delta = 2\,e^{-3/2}\left[1-4.002\sqrt{\delta}-7.717\delta\right]\text{(a.u.)}, \tag{17}$$

$$\Delta_m = \frac{4}{9}\left[1-\frac{13}{3}\sqrt{\delta}-8\delta\right]\text{(a.u.)}. \tag{18}$$

The factors $2e^{-3/2}$ and 4/9 refer to the hydrogen atom problem when $\delta=0$. The agreement between these coefficients is better than half a percent. The coefficients of $\sqrt{\delta}$ agree within 8% whereas those of δ agree within 4%. It is indeed satisfying to note that the agreement is so good for even the small correction factors. This is a reflection of the fact that our present approach has all the essential ingredients built into it.

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